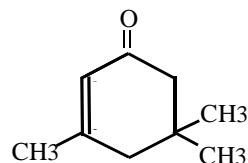


ISOPHORONE

Isophorone is a federal hazardous air pollutant and was identified as a toxic air contaminant in April 1993 under AB 2728.

CAS Registry Number: 78-59-1

Molecular Formula: $C_9H_{14}O$



Isophorone is a clear liquid with a peppermint, camphor odor. It is flammable and explosive when exposed to heat or flame and can react with oxidizing materials. Isophorone is soluble in alcohol, ether, and acetone and miscible in organic solvents (HSDB, 1991).

Physical Properties of Isophorone

Synonyms: isoacetophorone; 1,1,3-trimethyl-3-cyclohexene-5-one

Molecular Weight:	138.23
Boiling Point:	214 °C at 754 mm Hg
Melting Point:	-8.1 °C
Flash Point:	184 °F
Vapor Pressure:	0.38 mm Hg at 20 °C
Vapor Density:	4.77 (air = 1)
Density/Specific Gravity:	0.9229 at 20 °C (water = 1)
Log/Octanol Water Partition Coefficient:	1.7
Water Solubility:	12,000 mg/L at 25 °C
Henry's Law Constant:	5.8×10^{-6} atm-m ³ /mole
Conversion Factor:	1 ppm = 5.65 mg/m ³

(HSDB, 1991; Sax, 1989; U.S. EPA, 1994a)

SOURCES AND EMISSIONS

A. Sources

Isophorone is used as a solvent for lacquers, inks, vinyl resins, copolymers, coatings, and pesticides. It is also used as an intermediate in the manufacture of 3,5-xyleneol, 3,3,5-trimethylcyclohexanol. Coal fly ash is also a source of isophorone (HSDB, 1991).

The primary stationary sources that have reported emissions of isophorone in California are coating, engraving and allied services, public order and safety installations, and ship and boat building facilities (ARB, 1997b).

B. Emissions

The total emissions of isophorone from stationary sources in California are estimated to be at least 1,300 pounds per year, based on data reported under the Air Toxics “Hot Spots” Program (AB 2588) (ARB, 1997b).

C. Natural Occurrence

No information about the natural occurrence of isophorone was found in the readily-available literature.

AMBIENT CONCENTRATIONS

No Air Resources Board data exist for ambient measurements of isophorone.

INDOOR SOURCES AND CONCENTRATIONS

No information about the indoor sources and concentrations of isophorone was found in the readily-available literature.

ATMOSPHERIC PERSISTENCE

Based on its vapor pressure, isophorone is expected to exist primarily in the vapor phase in the troposphere. Isophorone is expected to react with hydroxyl (OH) radicals, nitrate (NO₃) radicals, and ozone (O₃). Rate constants for these reactions have not been measured to date, however, the OH radical reaction may dominate as a tropospheric loss process. Based on the estimated rate constants for the OH radical reaction (Greene and Atkinson, 1994), the calculated half-life and lifetime of isophorone due to reaction with the OH radical are 3.1 hours and 4.5 hours, respectively (Atkinson, 1995). Isophorone emitted to the atmosphere in particulate form may be removed by wet or dry deposition (Howard, 1990).

AB 2588 RISK ASSESSMENT INFORMATION

Although isophorone is reported as being emitted in California from stationary sources no health values (cancer or non-cancer) are listed in the California Air Pollution Control Officers Association Air Toxics “Hot Spots” Program Revised 1992 Risk Assessment Guidelines for use in risk assessments (CAPCOA, 1993).

HEALTH EFFECTS

Probable routes of human exposure to isophorone are inhalation, ingestion, and dermal contact.

Non-Cancer: Acute overexposure to isophorone in humans has been reported to cause

irritation of the skin, eyes, nose, and throat. At higher exposures, nausea and headache have also been reported. Workers chronically exposed to isophorone have been reported to develop dizziness, fatigue, and depression.

The United States Environmental Protection Agency (U.S. EPA) has determined that there are inadequate data for establishing a Reference Concentration (RfC) for isophorone, but has set the oral Reference Dose (RfD) at 0.2 milligrams per kilogram per day based on no-observed effects in dogs. The U.S. EPA estimates that consumption of this dose or less, over a lifetime, would not likely result in the occurrence of chronic, non-cancer effects (U.S. EPA, 1994a).

No information was located regarding adverse reproductive or developmental effects in humans. Limited evidence in animal studies suggests that inhalation exposure to isophorone during pregnancy may cause birth defects such as fetal malformations and growth retardation (U.S. EPA, 1994a).

Cancer: No studies were found concerning the carcinogenicity of isophorone in humans. In one animal study, an increased incidence of kidney tumors and preputial gland tumors in male rats was observed. The U.S. EPA has classified isophorone in Group C: Possible human carcinogen and has calculated an oral unit risk estimate of 2.7×10^{-8} (microgram per liter)⁻¹. The U.S. EPA estimates that if an individual were to ingest water containing isophorone at 40 micrograms per liter over an entire lifetime, that person would theoretically have no more than a 1 in 1 million increased chance of developing cancer. (U.S. EPA, 1994a). The International Agency for Research on Cancer (IARC) has not classified isophorone as to its human carcinogenicity (IARC, 1987a).

